WEB-BASED DATA EXCHANGE SYSTEM IN CHEMICAL PROCESS ENGINEERING

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ABSTRACT

Chemical engineering process is a very complex task. Fortunately, there are many different types of computer-aided system that have been developed used in chemical process activities. These software packages have improved chemical engineering design enormously and enabled process engineers to optimize design strategies and plant performance. However, the software packages generated and used different type of data. Therefore, these individual systems can not share the data fed to, and generated by, other application systems. A lot of time is spent on transferring the data manually from one application to another. The manual data transfer is time consuming and error-prone. Globalization makes the communication around the world becomes paramount nowadays. It is essential for engineers to exchange or sharing information around the world. This paper presents the exploration and implementation of the new technology – eXtensible Markup Language (XML) in chemical process engineering. XML is used as the neutral file format for data exchange to solve the problems above. XML file format is a very powerful data exchange format because it is platform-independent, self-describing and the data can be shared between programs without coordination. A web-based client/server data access will be developed to demonstrate the potential and benefits of the XML and Internet in chemical process engineering.

Keywords: chemical engineering data, data exchange, neutral file format, XML, Web

BACKGROUND

In chemical process engineering, the activities are so varied and diversified such as process synthesis, flow-sheet calculation, process optimization, plant design, dynamic simulation and control, equipment design and so on. Fortunately, the development and implementation of computer software packages helps the engineers to improve the design efficiency enormously and optimize design strategies and plant performance. However, the implementation of various types of software packages causes many different types of engineering information and data being generated. Moreover, these application systems are mostly stand-alone, which cannot share the data, fed to, and generated by, these or other application systems. A lot of time was spent on manually transfer the data from one application to another. The manual data transfer is time consuming and error-prone

The globalization makes the communication become paramount nowadays. Many chemical companies have built their chemical plants all over the world. The communication between headquarters and the sites is vital. Moreover, most of the front-end work is done in headquarter or in the research and development center. For more efficient performance, it is essential to allow the engineers to access the central database management system in headquarter from other side of the world for important information. Moreover, the world is becoming increasingly a closer-knit planet. It is typical to have people in various and diverse locations working on a single project. There is also a need to share or exchange the information from one system to another or share the engineering information with the experts around the world.

DATA SHARING

There are some applications, which can share data in existence today. Figure 1 shows the closed situation about these applications. Each application contents a customized point-to-point translator, which function as a bridge to share data between the applications. The translator must know about how to share the data between two different applications. In many cases, a bridge might not exist at all because most applications are using proprietary formats [1]. If the bridge exists, it grows quickly with the number of the systems, about the square of the number of systems (N*N-N). For example, 6 different systems need 30 point-to-point translators to share data among them.

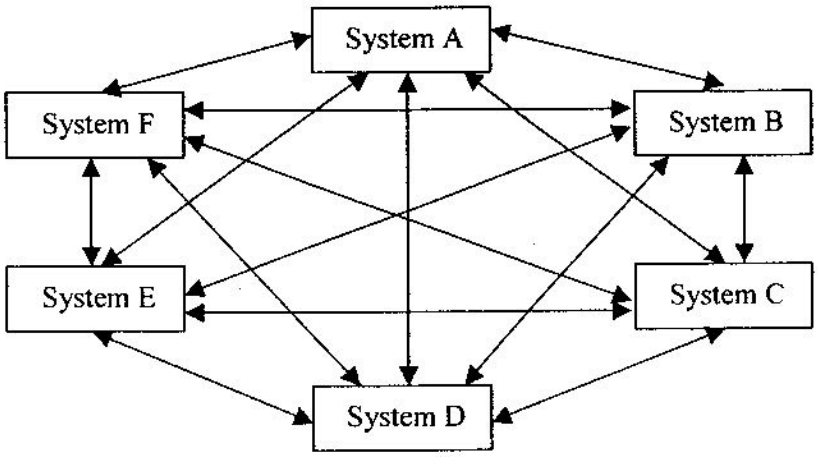

Figure 1 Point-to-point translator

The situation will become simpler, if a neutral file format is implemented. As shows in Figure 2, the neutral file is a common file, which can be shared by each application. Only a translator is needed for each system to translate the internal file format to or from the neutral file format.

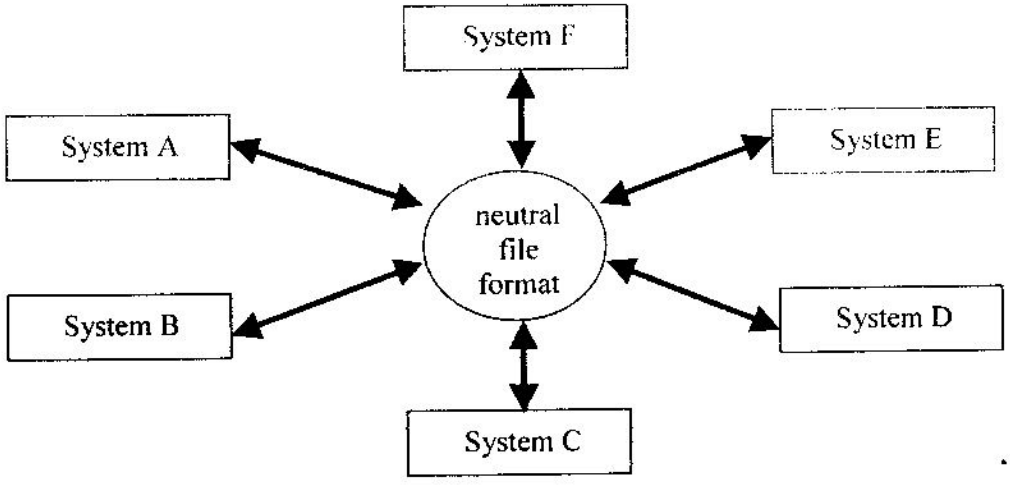

Figure 2 Neutral file format

XML

XML is one of the latest technologies in communication and information system. Development of XML started in 1996 and it is a W3C [2], the World Wide Web Consortium standard since February 1998. It is the simplified subset of SGML (Standard Generalized Markup Language. ISO 8897) optimized for delivery over the Web.

XML is a markup language. "Markup" is a method of conveying metadata, the information about the dataset. It means that every data in the XML is self-describing, which use string literals, or "tags", to delimit and describe the data. Moreover, XML is platform-independent which can be used to exchange data with other users and programs. Additionally, the data in XML can be shared between programs without coordination makes it very suitable to become the neutral file format for data exchange.

CHEMICAL PROCESS ENGINEERING DATA IN XML

Currently, most of the efforts are taken on the development of XML in the business application. For example, an XML based e-standard for chemical industry has been proposed by BASF, Dow Chemical, and DuPont, which was called "Data Exchange Standard for the Chemical Industry". It supports a general business-processing model such as customer/company information, product catalog, orders and envelope and security [3]. However, the XML capabilities are not limited only in the business applications. For example, XML has been implemented in biomedical engineering [4], medical informatics [5], geographic information systems [6] and so on. The potentials of XML have not been fully explored in engineering fields. It must be a big advantage if XML can be implemented in chemical process engineering.

Figure 3 shows the example of a part of chemical process simulation report from a simulator. The report shows the information about the operating conditions and the inlet and outlet of the hot stream conditions of a heat exchanger. This type of text file report format is totally unsuitable to use as a data exchange or sharing format. It is because the data and information in the file is difficult to be extracted and manipulated by the computer.

Figure 4 represents the chemical process simulation report in XML file. The file contains XML elements such as <heat_exchanger>, <operating_conditions>, <cold_side_conditions> and so on. Some of the elements contain attributes to describe the unit of the chemical process data such as M*KJ/HR for heat duty and KG-MOL/HR for mole flow rate and so on. The figure shows that the XML data is self-describing where the descriptive tags are intermixed with the data. The open and flexible format used by XML allows it to be employed wherever there is a need for the information exchange and transfer. This makes it extremely powerful for data exchange.

```
                                OUTPUT
                        HEAT EXCHANGER SUMMARY
================================================================================
                              UNIT 1, 'E1'

OPERATING CONDITIONS

     DUTY, M*KJ/HR                          49.640

COLD SIDE CONDITIONS                         INLET        OUTLET
                                          ----------   ----------
     FEED                                    S1
     VAPOR PRODUCT                                        S2
      VAPOR, KG-MOL/HR                                 1000.000
             K*KG/HR                                     46.069
          CP, KJ/KG-K                                     1.724
     LIQUID, KG-MOL/HR                    500.260
             K*KG/HR                       37.067
          CP, KJ/KG-K                       2.452
      WATER, KG-MOL/HR                    499.740
             K*KG/HR                       9.003
          CP, KJ/KG-K                       4.178
      TOTAL, KG-MOL/HR                   1000.000     1000.000
             K*KG/HR                       46.069       46.069
```

Figure 3 Example of chemical process simulation report

```
<?xml version='1.0'?>
<heat_exchanger id="E1">
        <operating_conditions>
                <duty unit="M*KJ/HR">49.640</duty>
                <cold_side_conditions>
                        <inlet stream="S1">
                                <vapor/>
                                <liquid>
                                        <mole unit="KG-MOL/HR">500.00</mole>
                                        <mass unit="K*KG/HR">37.067</mass>
                                        <cp unit="KJ/KG-K">2.452</cp>
                                </liquid>
                                <total>
                                        <mole unit="KG-MOL/HR">1000.00</mole>
                                        <mass unit="K*KG/HR">46.069</mass>
                                </total>
                        </inlet>
                        <outlet stream="S2">
                                <vapor>
                                        <mole unit="KG-MOL/HR">1000.00</mole>
                                        <mass unit="K*KG/HR">46.069</mass>
                                        <cp unit="KJ/KG-K">1.724</cp>
                                </vapor>
                                <liquid/>
                                <total>
                                        <mole unit="KG-MOL/HR">1000.00</mole>
                                        <mass unit="K*KG/HR">46.069</mass>
                                </total>
                        </outlet>
                </cold_side_conditions>
        </operating_conditions>
</heat_exchanger>
```

Figure 4 Example of chemical process data in XML file format

SYSTEM ARCHITECTURE

In the near future, the popular application software will have the ability to save information as XML. However, until this becomes the norm, a custom translator, which can convert the legacy format to XML, is needed to aggregating the disparate data. The translator must perform three functions, extraction through proprietary interfaces, transformation into XML, and packaging for transmission [7].

In Figure 5 shows the overall system architecture. The system contains many components: XML generator, HTML generator, translator, data filter and data extractor. The system not only provides the services of exchange data locally but also through the Internet. The information in the XML format is readable by the common Web browser. The users from every side of the world can refer the information from the Web site or even download it for their applications.

Figure 6 demonstrates a part of the system developed. The application is known as XML generator, which developed using Java programming language. At the back of the application, a simple database is developed to test the ability of the application to extract the data from the database. As shown in the figure, all the information about the process stream are extracted and displayed from the database. The users can filter and select the information about the chemical process stream they need from the list. Finally the filtered data will be converted into XML as show in the figure. The users are allowed to edit the generated XML. Finally, the save function is provided to save the file as XML file format.

The developed application demonstrates the data extraction and data filtration from a database. The application also shows how the data become a self-describing data in the XML file format. In the next phase of the research, more efforts will be taken on the implementation of XML file in chemical

engineering applications to demonstrate the powerful XML and how much the benefits of XML bring into the chemical engineering field.

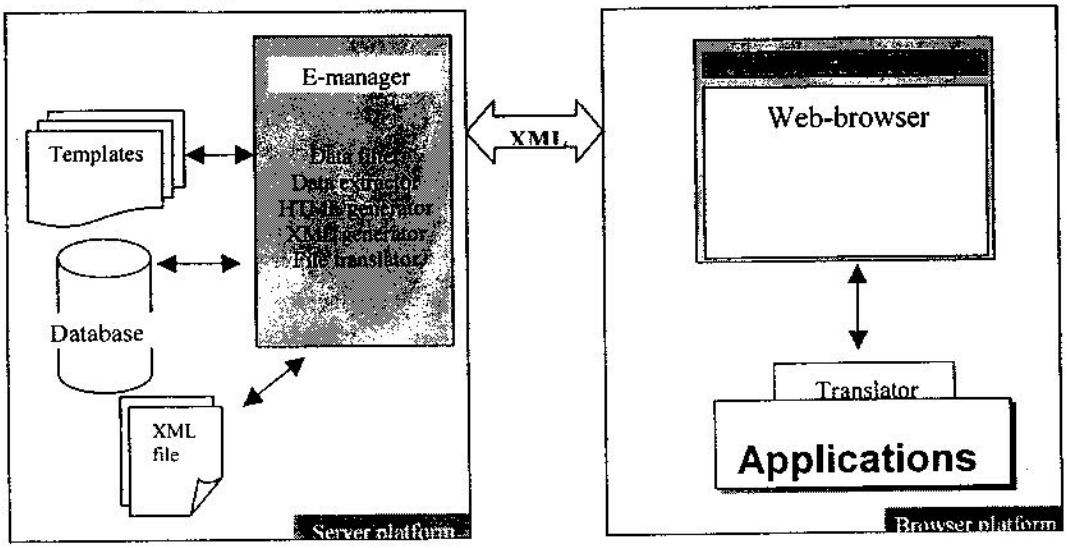

Figure 5 System Architecture

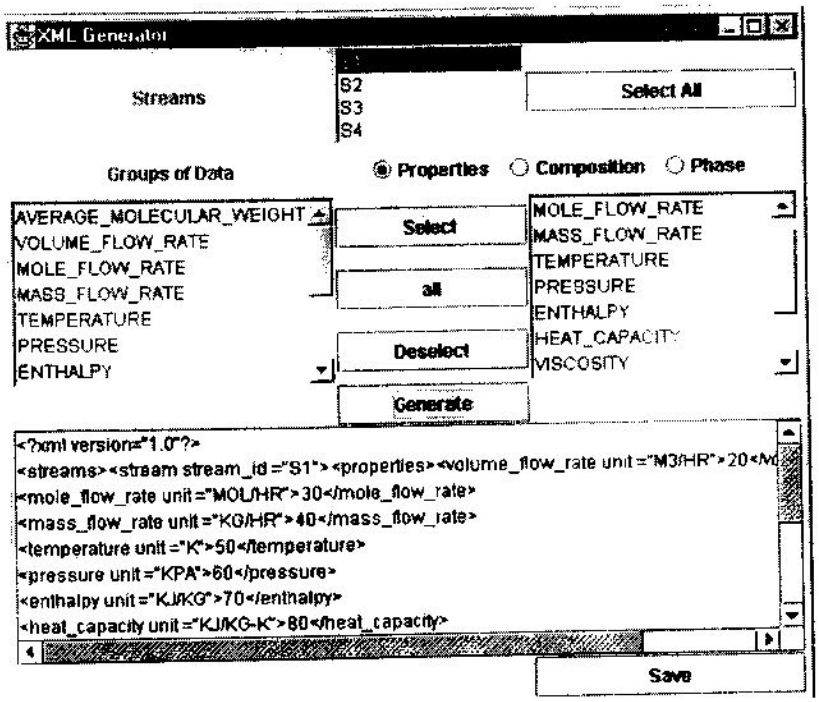

Figure 6 XML Generator

CONCLUSION

A perfect data exchange method provides a better design and increase the efficiency of engineers. For more effective data exchange in chemical process engineering, it is desired to implement the new technology of communication and information system. It is a first step for future development in this area.

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